



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 153496

TO: David Lukton
Location: REM-3B75/3C18
Art Unit: 1654
Monday, August 29, 2005

Case Serial Number: 09/600659

From: Edward Hart
Location: Biotech-Chem Library
REM-1A55
Phone: 571-272-2512

edward.hart@uspto.gov

Search Notes

Examiner Lukton,

Here are the results of the search you requested.

Please feel free to contact me if you have any questions.

Edward Hart

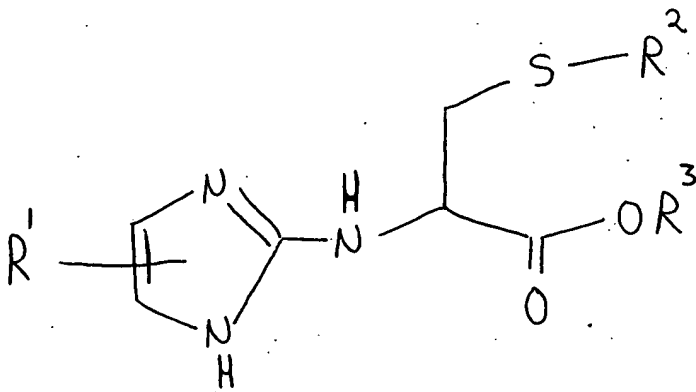
SEARCH REQUEST FORM
(STIC)

Requestor's Name: David Lukton Examiner number: 71263 Date: 7/6/05
Art Unit: 1654 Phone number: 571-272-0952 Serial Number: 09/600659
Mail Box: 3-C-18 Examiner Rm: 3-B-75 Results format: paper

Title: A PHARMACEUTICAL FORMULATION CONTAINING AN INHIBITOR OF
CARBOXYPEPTIDASE U AND A THROMBIN INHIBITOR

Applicants: ABRAHAMSSON, TOMMY; NERME, VIVECA; POLLA, MAGNUS

Earliest Priority Date: 5/3/99



R¹ = amino or alkylamino or amidino or guanidino;

R² = hydrogen or acyl;

R³ is anything;

STAFF USE ONLY

Type of Search

Vendors and cost where applicable

Searcher: _____ NA Sequence (#)

STN _____ Dialog

Searcher Phone #: _____ AA Sequence (#)

_____ Questel/Orbit _____ Lexis/Nexis

Searcher Location: _____ Structure (#)

_____ Westlaw _____ WWW/Internet

Date Searcher Picked Up: 8/1/05 _____ Bibliographic

_____ In-house sequence systems

Date Completed: _____ Litigation

_____ Commercial _____ Oligomer _____ Score/Length

Searcher Prep & Review Time: _____ Fulltext

_____ Interference _____ SPDI _____ Encode/Transl

Online Time: _____ Other

_____ Other (specify)

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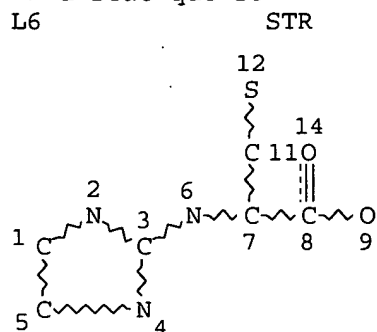
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FILE COVERS 1907 - 29 Aug 2005 VOL 143 ISS 10
 FILE LAST UPDATED: 28 Aug 2005 (20050828/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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 DEFAULT ECLEVEL IS LIMITED

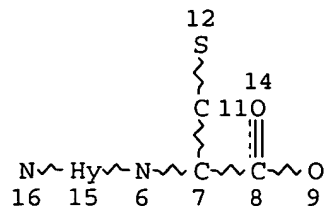
GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
 L8 0 SEA FILE=REGISTRY SSS FUL L6

100.0% PROCESSED 407 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

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L14 STR



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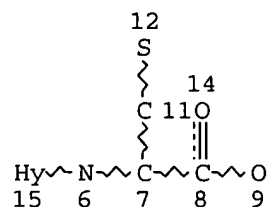
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STEREO ATTRIBUTES: NONE

L15 82 SEA FILE=REGISTRY SSS FUL L14

L18 STR



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GGCAT IS MCY AT 15

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L20 60 SEA FILE=REGISTRY SUB=L15 SSS FUL L18

L21 34 SEA FILE=HCAPLUS ABB=ON PLU=ON L20

L22 30 SEA FILE=HCAPLUS ABB=ON PLU=ON L21 AND PD<=MAY 3, 1999

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L22 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:318208 HCAPLUS

DOCUMENT NUMBER: 131:166490

TITLE: Root-exudated compounds as conjugation partners of pesticides in the rhizosphere

AUTHOR(S): Schneider, R. J.

CORPORATE SOURCE: Institut fur Agrikulturchemie Universitat Bonn, Bonn, D - 53115, Germany

SOURCE: Pflanzenernaehrung, Wurzeleistung und Exsudation, Borkheider Seminar zur Oekophysiologie des

Wurzelraumes, 8th, Schmerwitz, Germany, Sept. 22-24, 1997 (**1998**), Meeting Date 1997, 213-220.

Editor(s): Merbach, Wolfgang. Teubner: Stuttgart, Germany.

CODEN: 67RDAF

DOCUMENT TYPE:

Conference

LANGUAGE:

German

AB The formation of bound residues from pesticides in soil is still poorly understood. We assume that low mol. substances exudated from the roots of living plants are potential reaction partners for xenobiotic mols. in the rhizosphere. A reaction of pesticides with low-mol. substances as amino acids, carboxylic acids and carbohydrates should be kinetically favored in regard to the relatively inert central regions of humic substances. Possible conjugates of the terbutylazine have been postulated and synthesized. First results on the occurrence of these metabolites are presented.

IT **239092-58-1P**

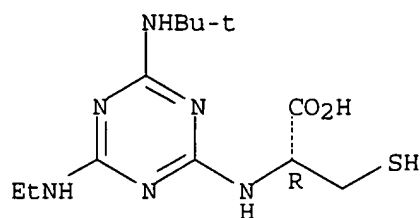
RL: AGR (Agricultural use); FMU (Formation, unclassified); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); USES (Uses)

(preparation as model for pesticide conjugates with rhizospheric root exudates)

RN 239092-58-1 HCAPLUS

CN L-Cysteine, N-[4-[(1,1-dimethylethyl)amino]-6-(ethylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:471284 HCAPLUS

DOCUMENT NUMBER: 129:171820

TITLE: The metabolism of atrazine and related 2-chloro-4,6-bis(alkylamino)-s-triazines in plants

AUTHOR(S): Lamoureux, Gerald L.; Simoneaux, Bruce; Larson, John

CORPORATE SOURCE: Biosciences Research Laboratory, ARS, USDA, State University Station, Fargo, ND, 58105-5674, USA

SOURCE: ACS Symposium Series (**1998**), 683(Triazine Herbicides: Risk Assessment), 60-81

CODEN: ACSMC8; ISSN: 0097-6156

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The metabolism of atrazine and related 2-chloro-4,6-bis(alkylamino)-s-triazine herbicides in plants is summarized and the structures of 13 metabolites recently identified from mature plants grown in the field are reported. The 2-chloro-4,6-bis(alkylamino)-s-triazines are initially metabolized in

plants by 3 competing reactions: hydrolytic dehalogenation, N-dealkylation, and glutathione (GSH) conjugation. Metabolites produced by N-dealkylation can be further metabolized by hydrolytic dehalogenation or GSH conjugation, those produced by hydrolytic dehalogenation can be further metabolized by N-dealkylation and it is proposed that those from the GSH conjugation pathway may slowly become hydroxylated at the 2-position of the triazine ring. Ten metabolites of atrazine have been identified from the N-dealkylation and hydroxylation pathways and 14 have been identified from the GSH conjugation pathway. Three addnl. metabolites that have an amino function on the 2-position of the triazine ring have been identified, but their route of formation is uncertain.

IT 211558-12-2 211558-13-3 211558-14-4

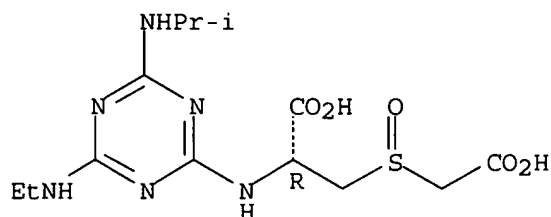
211558-15-5 211558-16-6

RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(atrazine metabolite in sugarcane)

RN 211558-12-2 HCAPLUS

CN L-Alanine, 3-[(carboxymethyl)sulfinyl]-N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

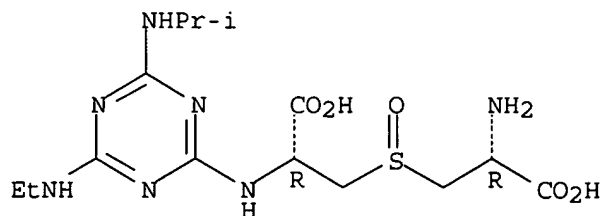
Absolute stereochemistry.



RN 211558-13-3 HCAPLUS

CN L-Alanine, 3-[[[(2R)-2-amino-2-carboxyethyl]sulfinyl]-N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

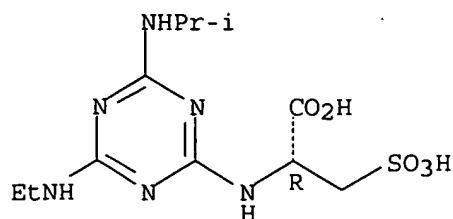
Absolute stereochemistry.



RN 211558-14-4 HCAPLUS

CN L-Alanine, N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]-3-sulfo- (9CI) (CA INDEX NAME)

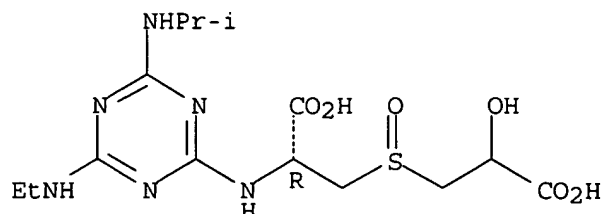
Absolute stereochemistry.



RN 211558-15-5 HCAPLUS

CN L-Alanine, 3-[(2-carboxy-2-hydroxyethyl)sulfinyl]-N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

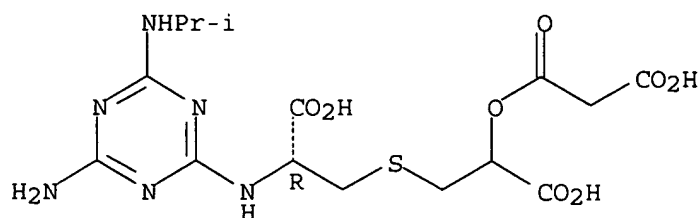
Absolute stereochemistry.



RN 211558-16-6 HCAPLUS

CN Propanedioic acid, mono[2-[[[(2R)-2-[[4-amino-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]amino]-2-carboxyethyl]thio]-1-carboxyethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:635209 HCAPLUS

DOCUMENT NUMBER: 125:250609

TITLE: Magenta recording fluids for ink-jet recording with good water resistance

INVENTOR(S): Satoh, Nobuyoshi; Hirasa, Takashi; Murata, Yukichi

PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan

SOURCE: PCT Int. Appl., 39 pp.

CODEN: PIXXD2

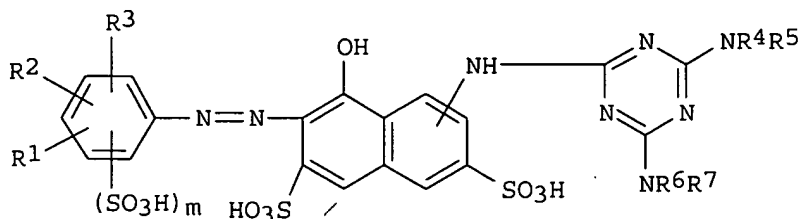
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

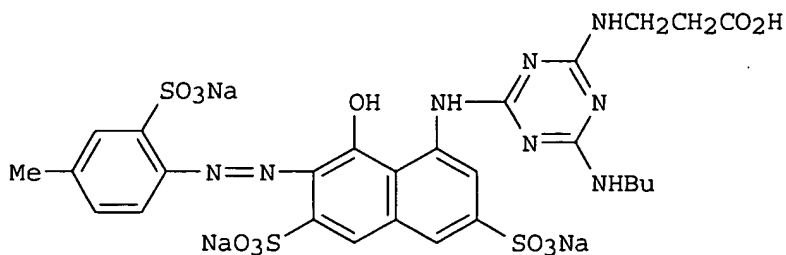
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9626985	A1	19960906	WO 1995-JP336	19950302 <--
W: US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 758672	A1	19970219	EP 1995-910729	19950302 <--
EP 758672	B1	20020731		
R: DE, GB				
US 5713992	A	19980203	US 1997-732451	19970113 <--
PRIORITY APPLN. INFO.:			WO 1995-JP336	W 19950302
OTHER SOURCE(S):		MARPAT 125:250609		
GI				



I



II

AB The title fluids comprise an aqueous medium and ≥ 1 monoazo dye I in free-acid form [R1-3 = H, (un)substituted C1-C9 alkyl, alkoxy, halogen, OH, (un)substituted carbamoyl, sulfamonyl, amino, nitro, sulfonic ester, sulfonyl, COOH, or carboxylic ester group; m = 0-2; R4-7 = H, C1-C18 alkyl, alkenyl, aryl, aralkyl, alicyclic or heterocyclic group, provided that all of the above non-H groups may be substituted and that ≥ 1 of R4-7 is substituted by COOH]. A fluid from diethylene glycol 10, iso-PROH 3, II 3, and water to 100 parts, adjusted to pH 9 by aqueous ammonia provided light- and wetfast jet prints on copying paper.

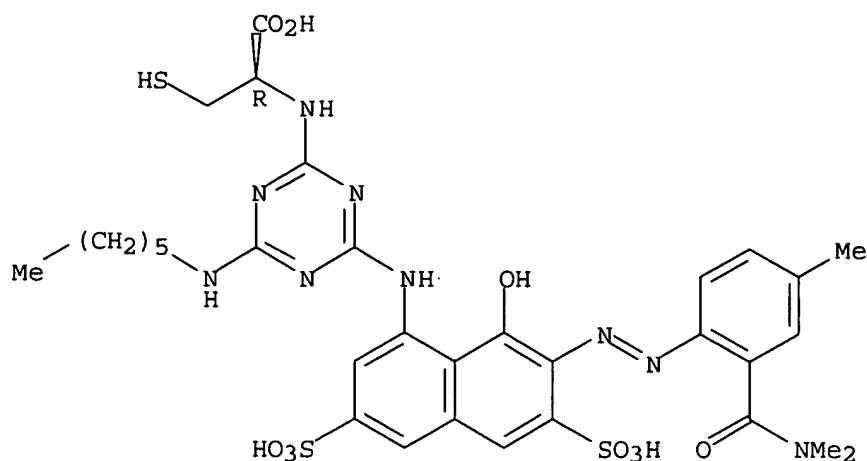
IT 182307-47-7

RL: TEM (Technical or engineered material use); USES (Uses)
(magenta recording fluids for ink-jet recording with good water resistance)

RN 182307-47-7 HCAPLUS

CN L-Cysteine, N-[4-[[7-[[2-[(dimethylamino)carbonyl]-4-methylphenyl]azo]-8-hydroxy-3,6-disulfo-1-naphthalenyl]amino]-6-(hexylamino)-1,3,5-triazin-2-yl]-, disodium salt (9CI) (CA INDEX NAME)

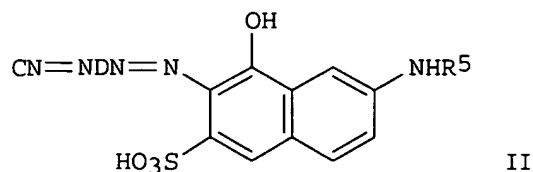
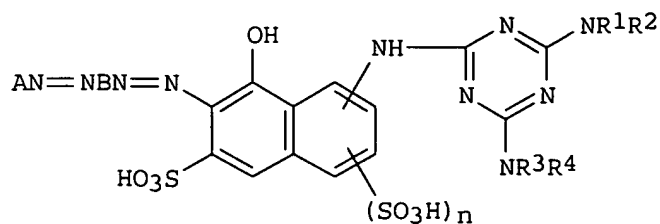
Absolute stereochemistry.
Double bond geometry unknown.



● 2 Na

L22 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:169303 HCAPLUS
 DOCUMENT NUMBER: 124:263652
 TITLE: Water-based black recording liquids containing azo dyes
 INVENTOR(S): Sano, Hideo; Yamada, Masahiro; Nishimura, Tooru; Takimoto, Hiroshi
 PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07331145	A2	19951219	JP 1994-125100	19940607 <--
JP 3371542	B2	20030127		
PRIORITY APPLN. INFO.:			JP 1994-125100	19940607
OTHER SOURCE(S):	MARPAT 124:263652			
GI				



AB Title liqs., useful for ink-jet printing black inks, etc., contain aqueous medium and ≥ 1 I-type azo dye and ≥ 1 II-type azo dyes [as free acids; A, C = (substituted) Ph, (substituted) naphthyl; B, D = (substituted) phenylene, (substituted) naphthylene; R1-5 = H, C1-18 alkyl, C1-18 alkenyl, aryl, aralkyl, cycloalkyl, heterocycle; which may be substituted; ≥ 1 R1-4 are carboxyl-substituted; n = 0-1]. The liqs. may comprise water 35-93, water-soluble organic solvents 5-50, and the dyes 2-8%.

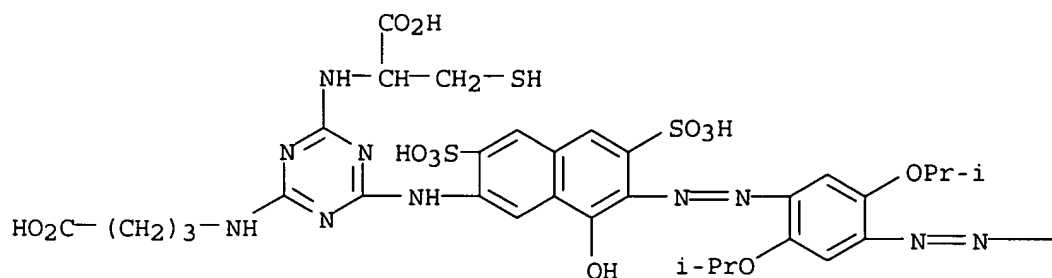
IT 175466-11-2

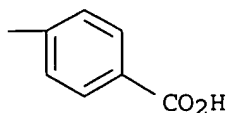
RL: TEM (Technical or engineered material use); USES (Uses)
(black water-based jet printing inks containing disazo dyes)

RN 175466-11-2 HCAPLUS

CN Benzoic acid, 4-[[[4-[[7-[[4-[(1-carboxy-2-mercaptoethyl)amino]-6-[(3-carboxypropyl)amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]-2,5-bis(1-methylethoxy)phenyl]azo]- (9CI) (CA INDEX NAME)

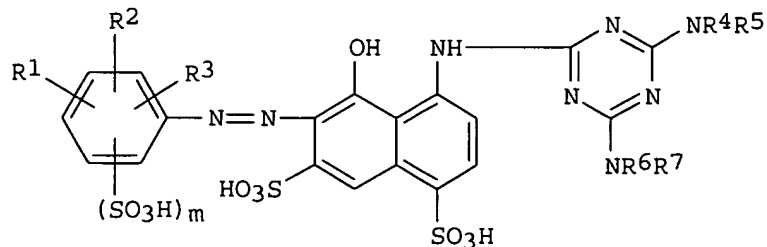
PAGE 1-A





L22 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:35311 HCAPLUS
 DOCUMENT NUMBER: 124:90619
 TITLE: Ink-jet printing liquids containing triazine-substituted azo magenta dyes
 INVENTOR(S): Sano, Hideo; Murata, Jukichi
 PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07278478	A2	19951024	JP 1994-72186	19940411 <--
JP. 3440544	B2	20030825		
PRIORITY APPLN. INFO.:			JP 1994-72186	19940411
OTHER SOURCE(S):	MARPAT 124:90619			
GI				



I

AB Title inks contain water-based mediums and I [R1-R3 = C1-9 (substituted) alkyl, C1-9 alkoxy, halo, H, OH, (substituted) carbamoyl, (substituted) sulfamoyl, (substituted) amino, NO2, sulfonate ester, SO2, CO2H, carboxylate ester; R4-R7 = H, C1-18 (substituted) alkyl, (substituted) alkenyl, aryl, aralkyl, alicyclic or heterocyclic group; m = 0-2]. The

inks provide magenta printed image with high color d., good light and water resistance. Thus, an ink containing I (R1 = p-Me; o-SO₃Na; R2-R6 = H; R5 = C₂H₄CO₂H; R7 = Bu; Na salt), diethylene glycol, iso-Pr alc., and water was subjected to ink-jet printing onto electrophotog. printing paper.

IT 172852-74-3

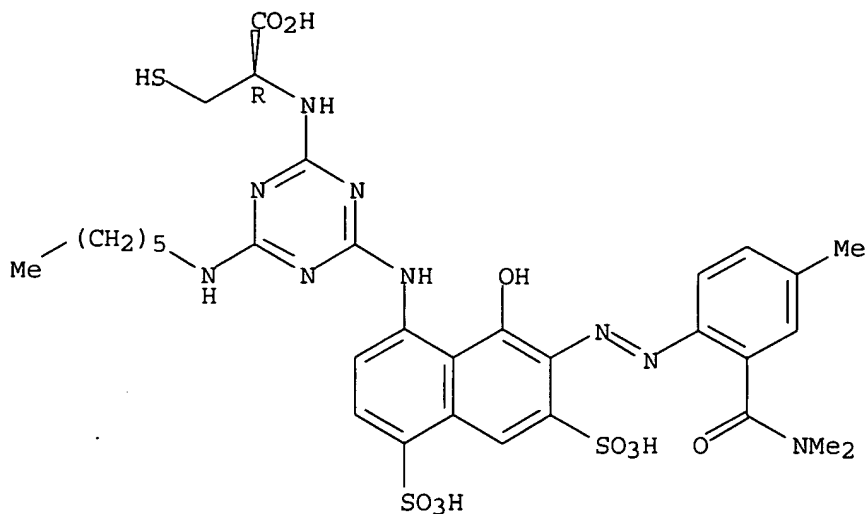
RL: TEM (Technical or engineered material use); USES (Uses)
(dyes; water-based jet-printing inks containing triazine-substituted magenta azo dyes)

RN 172852-74-3 HCAPLUS

CN L-Cysteine, N-[4-[[7-[[2-[(dimethylamino)carbonyl]-4-methylphenyl]azo]-8-hydroxy-4,6-disulfo-1-naphthalenyl]amino]-6-(hexylamino)-1,3,5-triazin-2-yl]-, dilithium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A

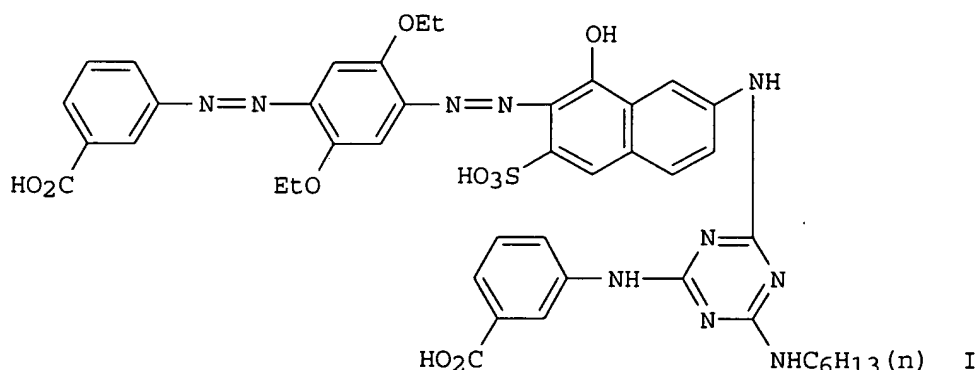


PAGE 2-A

● 2 Li

L22 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:867632 HCAPLUS
 DOCUMENT NUMBER: 123:260079
 TITLE: Jet-printing and writing inks
 INVENTOR(S): Sano, Hideo; Murata, Yukichi; Nishimura, Toru; Yamada, Masahiro; Takimoto, Hiroshi; Sato, Nobuyoshi
 PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan
 SOURCE: Eur. Pat. Appl., 47 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
EP 656407	A2	19950607	EP 1994-118779	19941129 <--
EP 656407	A3	19960710		
EP 656407	B1	19990303		
R: DE, FR, GB				
JP 07196967	A2	19950801	JP 1994-271413	19941104 <--
JP 3451755	B2	20030929		
JP 07207203	A2	19950808	JP 1994-271415	19941104 <--
JP 3484581	B2	20040106		
JP 07207204	A2	19950808	JP 1994-271416	19941104 <--
JP 3467533	B2	20031117		
JP 08113742	A2	19960507	JP 1994-271414	19941104 <--
JP 3428178	B2	20030722		
PRIORITY APPLN. INFO.:			JP 1993-298186	A 19931129
			JP 1993-301925	A 19931201
			JP 1993-301927	A 19931201
			JP 1994-202056	A 19940826
OTHER SOURCE(S):			MARPAT 123:260079	
GI				



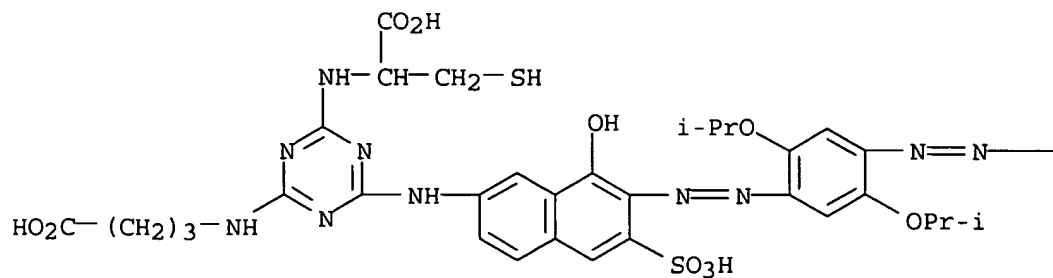
AB Storage-stable title inks that provide high-d. black images with good color tone and light and water resistance contain ≥ 1 dye selected from a series of dis- and trisazo acid dyes, some of which contain triazine groups. A typical aqueous ink with pH 9 contained diethylene glycol 10, iso-PrOH 3, and disazo dye I 3 parts.

IT **169195-81-7 169195-92-0**
 RL: TEM (Technical or engineered material use); USES (Uses)
 (dye; storage-stable jet-printing and writing inks containing acid dis- or trisazo dyes and providing high-d. black images with good color tone and light and water resistance)

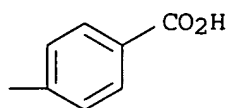
RN 169195-81-7 HCAPLUS

CN Benzoic acid, 4-[[4-[[7-[[4-[(1-carboxy-2-mercaptoethyl)amino]-6-[(3-carboxypropyl)amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3-sulfo-2-naphthalenyl]azo]-2,5-bis(1-methylethoxy)phenyl]azo]- (9CI) (CA INDEX NAME)

PAGE 1-A

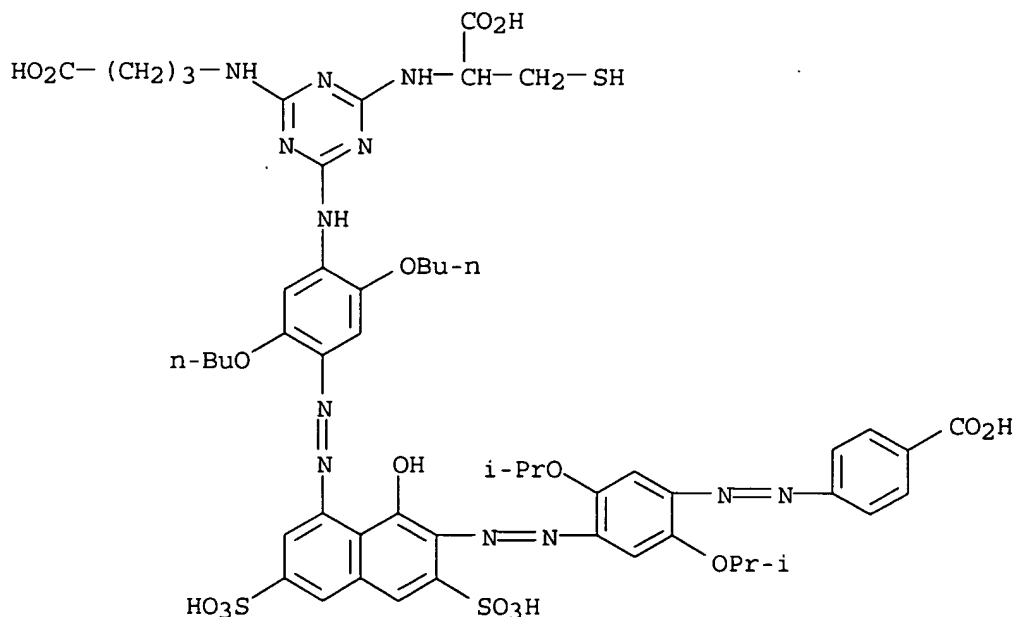


PAGE 1-B



RN 169195-92-0 HCAPLUS

CN Benzoic acid, 4-[[[4-[[[8-[[2,5-dibutoxy-4-[[4-[(1-carboxy-2-mercaptoethyl)amino]-6-[(3-carboxypropyl)amino]-1,3,5-triazin-2-yl]amino]phenyl]azo]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]-2,5-bis(1-methylethoxy)phenyl]azo]- (9CI) (CA INDEX NAME)

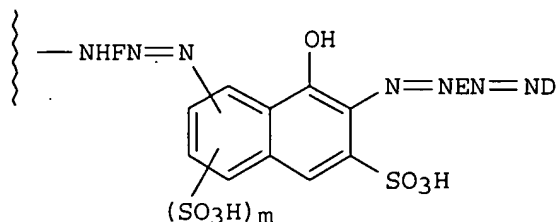
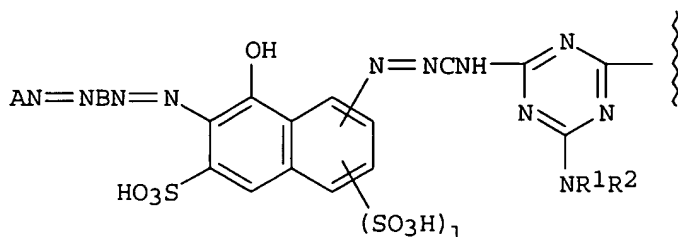


L22 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:804804 HCAPLUS
 DOCUMENT NUMBER: 123:343748

TITLE: Recording liquids containing tetraazo dyes
 INVENTOR(S): Sano, Hideo; Sato, Nobuyoshi; Murata, Jukichi
 PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07173422	A2	19950711	JP 1993-322244	19931221 <--
PRIORITY APPLN. INFO.:			JP 1993-322244	19931221
OTHER SOURCE(S):	MARPAT	123:343748		

GI



I

AB Title liqs., useful for ink-jet printing, contain water-based mediums and colorants comprising tetraazo compds., as free acids, I [A, D = (substituted) Ph, naphthyl; B, C, E, F = (substituted) phenylene, naphthylene; R1, R2 = H, C1-18 (substituted) alkyl, C1-18 (substituted) alkenyl, C1-18 (substituted) alkenyl, (substituted) aryl, (substituted) cycloalkyl, (substituted) aralkyl, (substituted) heteocycle; 1, m = 0, 1]. Thus, diethylene glycol 10, iso-Pr alc. 3, and tetraazo dye II 3 parts were mixed and blended with balance aqueous NH3 to give 100 parts ink, which was used for ink-jet printing to give images with water resistance and prevention of blurring.

IT 170442-31-6

RL: TEM (Technical or engineered material use); USES (Uses)
 (aqueous ink-jet printing inks containing tetraazo dyes)

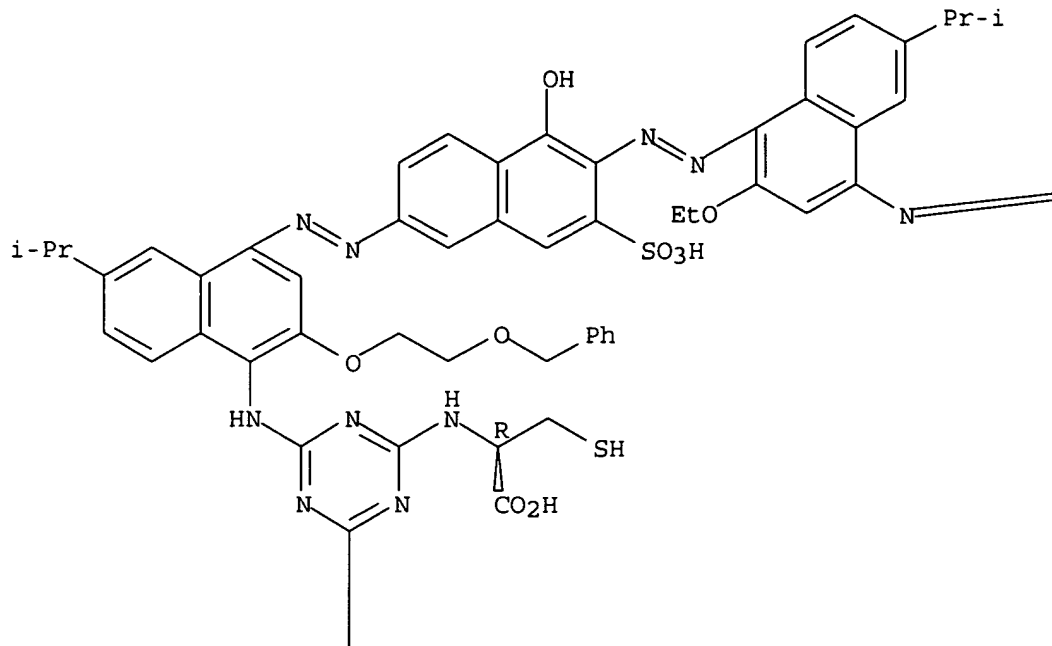
RN 170442-31-6 HCAPLUS

CN L-Cysteine, N-[4-[[4-[[6-[[4-[(4,8-disulfo-2-naphthalenyl)azo]-2-ethoxy-6-(1-methylethyl)-1-naphthalenyl]azo]-5-hydroxy-7-sulfo-2-naphthalenyl]azo]-6-(1-methylethyl)-2-[2-(phenylmethoxy)ethoxy]-1-naphthalenyl]amino]-6-[[4-[[6-[[4-[(4,8-disulfo-2-naphthalenyl)azo]-2-ethoxy-5-(1-methylethyl)phenyl]azo]-5-hydroxy-7-sulfo-2-naphthalenyl]azo]-5-(1-

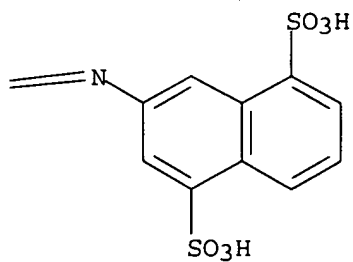
methylethyl)-2-[2-(phenylmethoxy)ethoxy]phenyl]amino]-1,3,5-triazin-2-yl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

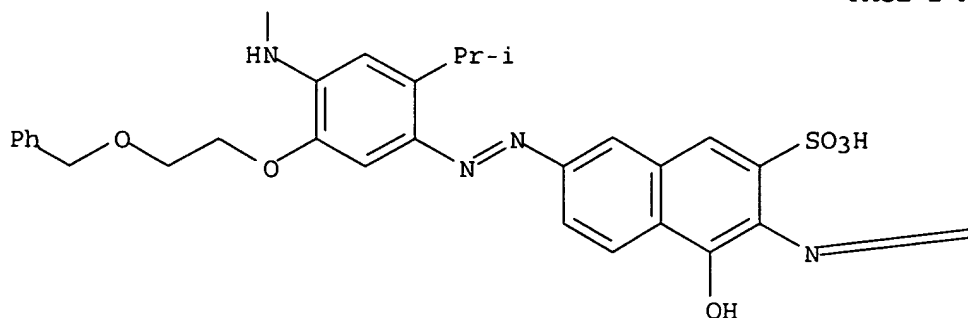
PAGE 1-A



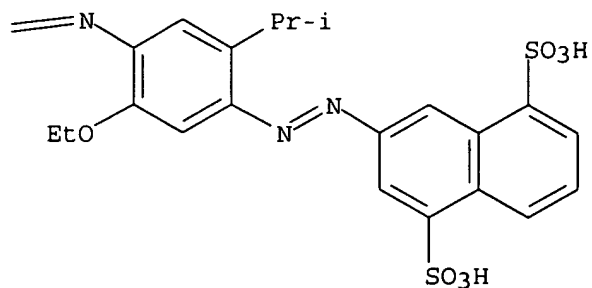
PAGE 1-B



PAGE 2-A



PAGE 2-B



L22 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:785207 HCAPLUS
 DOCUMENT NUMBER: 123:343739
 TITLE: Water-based recording liquids containing
 bistriazine-containing tetraazo dyes
 INVENTOR(S): Sano, Hideo; Sato, Nobuyoshi; Murata, Jukichi
 PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan; Mitsubishi Chemical Corp.
 SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07150088	A2	19950613	JP 1993-301926	19931201 <--
JP 3511652	B2	20040329		
PRIORITY APPLN. INFO.:			JP 1993-301926	19931201
OTHER SOURCE(S):	MARPAT 123:343739			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title liqs., useful for ink-jet printer, etc., contain water-based mediums and ≥ 1 dyes selected from tetraazo compds. I as free acids [A, D = (substituted) Ph, naphthyl; B, C = (substituted) phenylene, naphthylene; R1-4 = H, (substituted) C1-18 alkyl, (substituted) C1-18 alkenyl, (substituted) aryl, (substituted) aralkyl, (substituted) cycloalkyl, (substituted) heterocycle; Y = divalent linking group; m, n = 0, 1]. Thus, diethylene glycol 10, iso-Pr alc. 3, tetrazo dye II 3, and balance water were mixed to give title liquid providing clear bluish black dots in ink-jet printing.

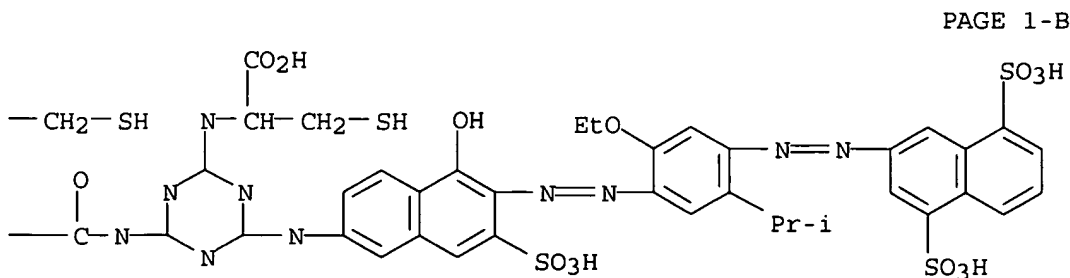
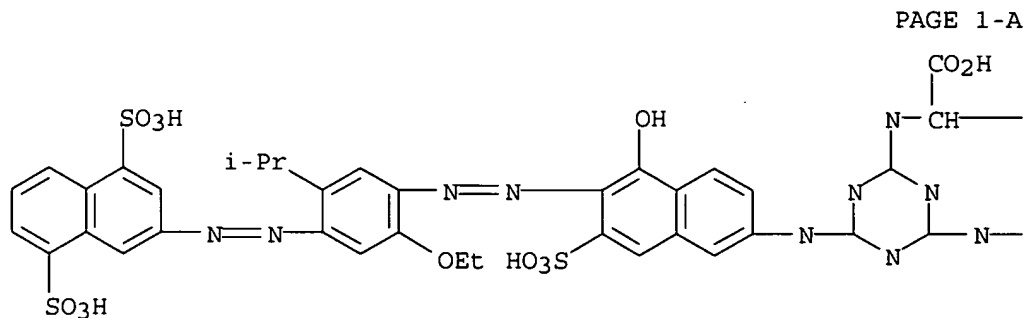
IT 170694-15-2

RL: TEM (Technical or engineered material use); USES (Uses)

(dyes; inks containing water-based mediums and bistriazine-containing tetraazo dyes)

RN 170694-15-2 HCAPLUS

CN L-Cysteine, N,N'-[carbonylbis[imino[6-[[6-[[4-[[4,8-disulfo-2-naphthalenyl)azo]-2-ethoxy-5-(1-methylethyl)phenyl]azo]-5-hydroxy-7-sulfo-2-naphthalenyl]amino]-1,3,5-triazine-4,2-diyl]]]bis- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L22 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:636369 HCAPLUS

DOCUMENT NUMBER: 123:290013

TITLE: Magenta ink solutions containing azo dyes with good

light and water resistance
 INVENTOR(S): Sato, Nobuyoshi; Hirasa, Takashi; Murata, Jukichi
 PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan; Mitsubishi Chemical Corp.
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07090212	A2	19950404	JP 1994-178355	19940729 <--
JP 3486966	B2	20040113		
PRIORITY APPLN. INFO.:			JP 1994-178355	A 19940729
			JP 1993-190045	19930730
OTHER SOURCE(S):	MARPAT 123:290013			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

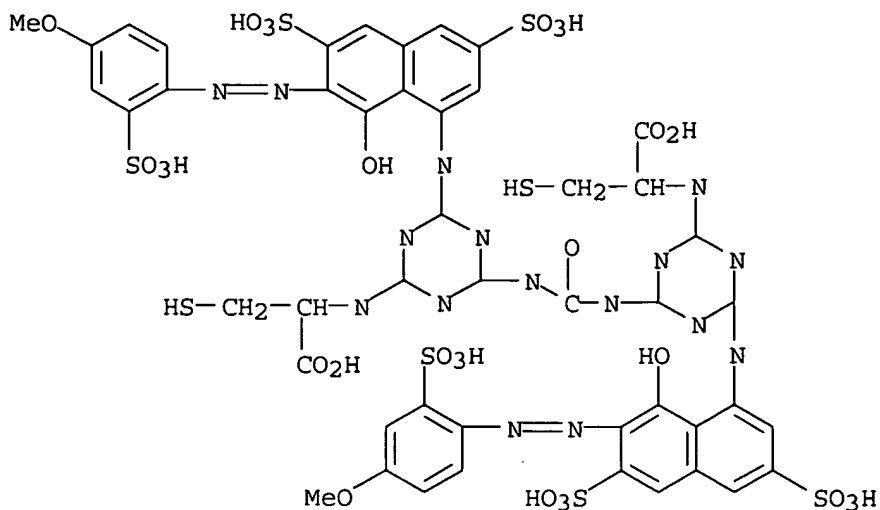
AB The title solns. useful for ink-jet printing, pens, etc., contain, in aqueous medium, azo dyes I [R1-R3, R8-R10 = C1-9 (un)substituted alkyl, C1-9 alkoxy, halogen, H, OH, (un)substituted carbamoyl, (un)substituted sulfamoyl, (un)substituted NH2, NO2, sulfonate ester residue, SO2, carboxylate ester residue; m, n = 0-2; R4-R7 = H, (un)substituted C1-18 alkyl, (un)substituted C1-18 alkenyl, (un)substituted aryl, (un)substituted aralkyl, (un)substituted alicyclyl, (un)substituted heterocyclyl; ≥1 of R4-R7 = 1-4 CO2H-substituted group; Y = divalent group] (as free forms). Thus, an ink containing 3% II was stable at 5 or 60° for 1 mo and provided storage-stable ink-jet prints.

IT **169754-39-6**
 RL: TEM (Technical or engineered material use); USES (Uses)
 (magenta ink solns. containing azo dyes with good light and water resistance)

RN 169754-39-6 HCAPLUS

CN L-Cysteine, N,N'-[carbonylbis[imino[6-[[8-hydroxy-7-[(4-methoxy-2-sulphophenyl)azo]-3,6-disulfo-1-naphthalenyl]amino]-1,3,5-triazine-4,2-diyl]]]bis-, hexapotassium salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

● 6 K

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L22 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:636368 HCAPLUS

DOCUMENT NUMBER: 123:290012

TITLE: Magenta ink solutions containing monoazo dyes with good light and water resistance

INVENTOR(S): Sato, Nobuyoshi; Hirasa, Takashi; Murata, Jukichi

PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan; Mitsubishi Chemical Corp.

SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.

CODEN: JKXXAF

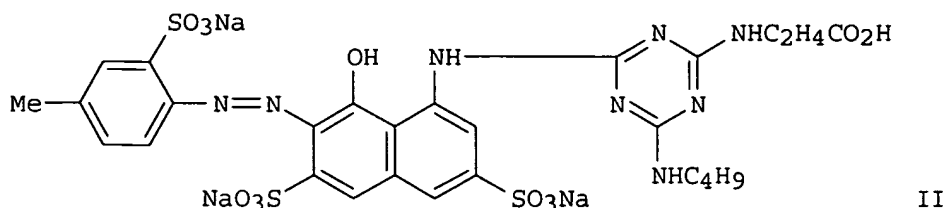
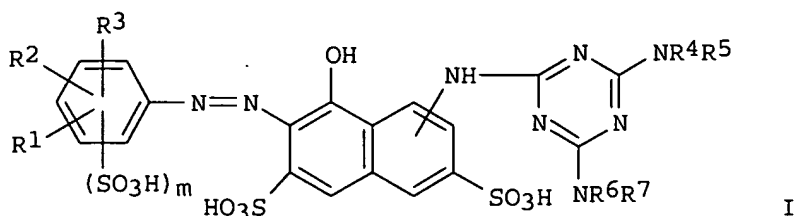
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07090211	A2	19950404	JP 1994-146514	19940628 <--
JP 3511677	B2	20040329		
PRIORITY APPLN. INFO.:			JP 1994-146514	A 19940628
			JP 1993-190044	19930730
OTHER SOURCE(S):		MARPAT 123:290012		
GI				



AB The title solns. useful for ink-jet printing, pens, etc., contain, in aqueous medium, monoazo dyes I [R1-R3 = C1-9 (un)substituted alkyl, C1-9 alkoxy, halogen, H, OH, (un)substituted carbamoyl, (un)substituted sulfamoyl, (un)substituted NH2, NO2, sulfonate ester residue, SO2, CO2H, carboxylate ester residue; m = 0-2; R4-R7 = H, (un)substituted C1-18 alkyl, (un)substituted C1-18 alkenyl, (un)substituted aryl, (un)substituted aralkyl, (un)substituted alicyclyl, (un)substituted heterocyclyl; ≥1 of R4-R7 = CO2H-substituted group] in free form. Thus, an ink containing 3% II was stable at 5 or 60° for 1 mo and provided storage-stable ink-jet prints.

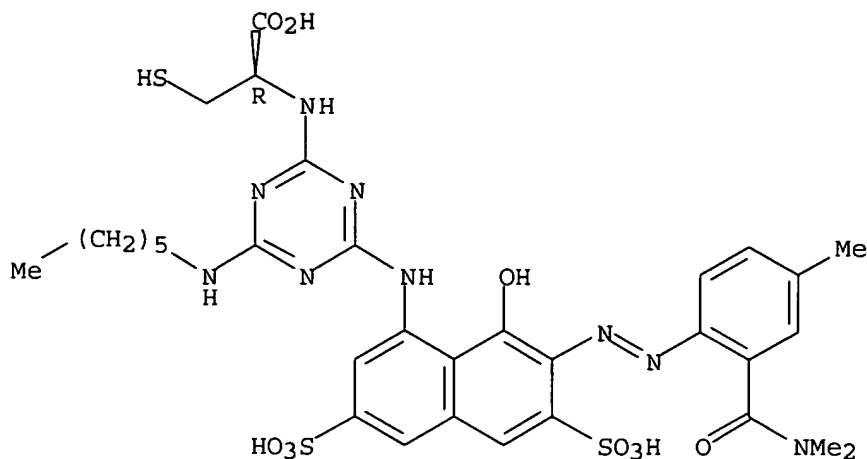
IT 169753-83-7

RL: TEM (Technical or engineered material use); USES (Uses)
(magenta ink solns. containing monoazo dyes with good light and water resistance)

RN 169753-83-7 HCAPLUS

CN L-Cysteine, N-[4-[[7-[[2-[(dimethylamino)carbonyl]-4-methylphenyl]azo]-8-hydroxy-3,6-disulfo-1-naphthalenyl]amino]-6-(hexylamino)-1,3,5-triazin-2-yl]-, dilithium salt (9CI) (CA INDEX NAME)

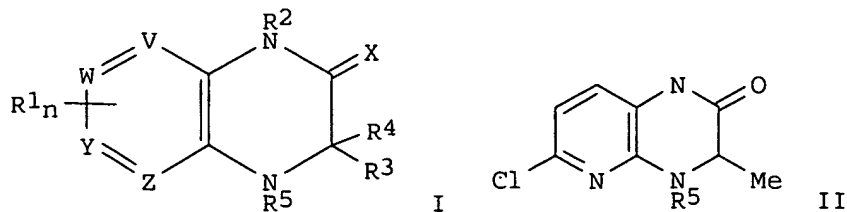
Absolute stereochemistry.
Double bond geometry unknown.



● 2 Li

L22 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1994:700922 HCAPLUS
 DOCUMENT NUMBER: 121:300922
 TITLE: Preparation of azaquinoxalinones as antiviral agents
 INVENTOR(S): Billhardt-Troughton, Uta Maria; Roesner, Manfred;
 Bender, Rudolf; Meichsner, Christoph
 PATENT ASSIGNEE(S): Hoechst A.-G., Germany
 SOURCE: Eur. Pat. Appl., 42 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 590428	A1	19940406	EP 1993-114934	19930916 <--
EP 590428	B1	19991215		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 187724	E	20000115	AT 1993-114934	19930916
ES 2141744	T3	20000401	ES 1993-114934	19930916
AU 9347553	A1	19940331	AU 1993-47553	19930923 <--
AU 664643	B2	19951123		
US 5424311	A	19950613	US 1993-125163	19930923 <--
IL 107081	A1	19990714	IL 1993-107081	19930923
CA 2106882	AA	19940327	CA 1993-2106882	19930924 <--
ZA 9307081	A	19940418	ZA 1993-7081	19930924 <--
HU 65302	A2	19940502	HU 1993-2696	19930924 <--
JP 06211855	A2	19940802	JP 1993-237679	19930924 <--
GR 3032520	T3	20000531	GR 2000-400216	20000131
PRIORITY APPLN. INFO.:			DE 1992-4232392	A 19920926
OTHER SOURCE(S):	MARPAT 121:300922			
GI				



AB Title compds. [tautomeric I; R1 = halo, CF3, OH, (cyclo)alkyl, alkoxy, Ph, etc.; R2,R5 = H, OH, alkyl, etc.; R3,R4 = H, (cyclo)alk(en)yl, (hetero)aryl, etc.; V,W,Y,Z = CH, CR1, N; X = O, S, NR2; n = 0-3] were prepared Thus, 2,6-dichloro-3-nitropyridine was condensed with L-H2NCHMeCO2Me and the reduced monocondensed product cyclized to give title compound (S)-II (R5 = H) which was reductively condensed with Me2CH:CHCHO to give (S)-II (R5 = CH2CH:CHMe2). The latter had MIC of 0.08µg/mL against HIV in cell culture.

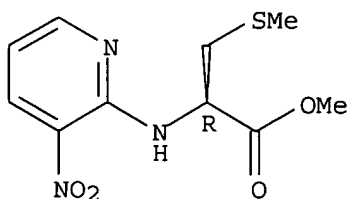
IT **159104-71-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antiviral agent)

RN 159104-71-9 HCAPLUS

CN L-Cysteine, S-methyl-N-(3-nitro-2-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L22 ANSWER 12 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:34091 HCAPLUS

DOCUMENT NUMBER: 108:34091

TITLE: Immobilization of urease from Staphylococcus saprophyticus L-1 on activated silicas

AUTHOR(S): Lyubinskii, G. V.; Yanishpol'skii, V. V.; Tertykh, V. A.; Juodvalkite, D.; Glemza, A.

CORPORATE SOURCE: Dep. Chem. Surf., L. V. Pisarzhevsky Inst. Phys. Chem., Kiev, USSR

SOURCE: Ukrainskii Biokhimicheskii Zhurnal (1978-1999) (1987), 59(4), 35-41

CODEN: UBZHD4; ISSN: 0201-8470

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The immobilization of urease obtained from *S. saprophyticus* L-1 on organic silica surfaces was studied. The process completion time (4-5 h) and the optimal pH of binding (7-8) are practically independent of the chemical nature of the carrier surface. The value of the specific activity of urease grafted to silica depends not only on the type of the enzyme-carrier bond, but also on the macromol. protein-to-silica distance. The extent of the retained enzyme activity is 26% after sorption on the

initial silica. It increases to 100% with an increase of the organic radical length which separates the biocatalyst and the carrier.

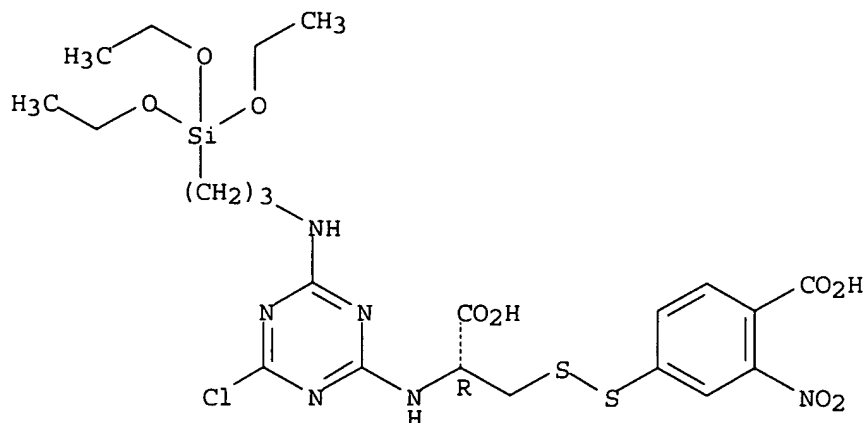
IT **112147-11-2DP**, derivs.

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and urease immobilization on)

RN 112147-11-2 HCAPLUS

CN Benzoic acid, 4-[[2-carboxy-2-[[4-chloro-6-[[3-(triethoxysilyl)propyl]amino]-1,3,5-triazin-2-yl]amino]ethyl]dithio]-2-nitro-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 13 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:104256 HCAPLUS

DOCUMENT NUMBER: 104:104256

TITLE: Amino acid conjugates of chloro-s-triazine: model substances for biodegradation study of s-triazine herbicides in plants

AUTHOR(S): Oluic-Vukovic, Vesna; Babic-Gojmerac, Tihomira; Mihanovic, Branka

CORPORATE SOURCE: Fac. Food Sci. Biotechnol., Univ. Zagreb, Zagreb, YU-41000, Yugoslavia

SOURCE: Journal of the Serbian Chemical Society (1985), 50(3), 121-4

CODEN: JSCSEN; ISSN: 0352-5139

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To improve the ability to follow the transformation process in plant tissue, 3 amino acid conjugates of chloro-s-triazine were synthesized as model substances and characterized by elemental anal., TLC, IR, and UV spectra. N,N'-Bis(4-chloro-6-ethylamino-s-triazin-2-yl)cystine [88552-50-5], one of the model substances, gave bis[β-(6-N-ethylamino-4-hydroxy-s-triazin-2-yl)aminoethyl]disulfide [100595-92-4] upon oxidation with H₂O₂. Two amino acid conjugates were tested for their herbicidal effect on oats (Avena sativa) in greenhouse expts. Both conjugates exhibited herbicidal activity.

IT **88552-50-5P 100595-91-3P**

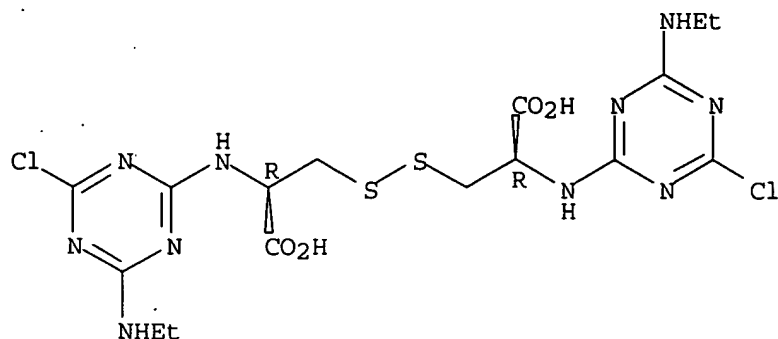
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and biodegrdn. of, by plants)

RN 88552-50-5 HCAPLUS

CN L-Cystine, N,N'-bis[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]- (9CI)

(CA INDEX NAME).

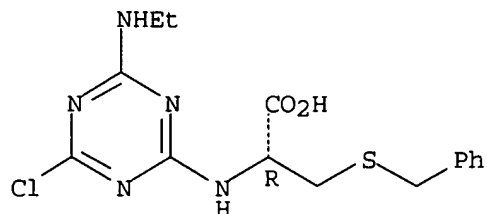
Absolute stereochemistry.



RN 100595-91-3 HCAPLUS

CN L-Cysteine, N-[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]-S-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1984:63390 HCAPLUS

DOCUMENT NUMBER: 100:63390

TITLE: Degradation of N,N'-bis(4-chloro-6-ethylamino-S-triazinyl-2)-cystine in buffered extract of cucumber seedlings (*Cucumis sativus*)

AUTHOR(S): Gojmerac, Tihomira

CORPORATE SOURCE: Fac. Technol., Univ. Zagreb, Zagreb, Yugoslavia

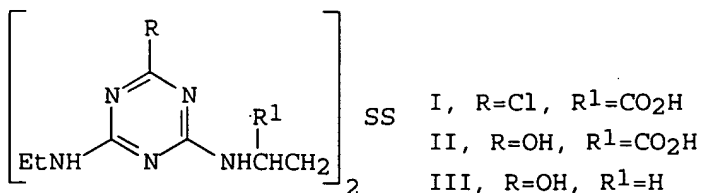
SOURCE: Fragmenta Herbológica Jugoslavica (1982), 11(2), 89-97

CODEN: FHJUDA; ISSN: 0350-3615

DOCUMENT TYPE: Journal

LANGUAGE: Serbo-Croatian

GI



AB Ten-day-old cucumber seedlings were extracted with pH 6.98 phosphate buffer and the extract was incubated with the title triazine-cystine conjugate I [88552-50-5] at 4° for 2 wk. The following pathway of I metabolism was determined: I + 2H₂O → II [88552-51-6] - 2CO₂ → III [88552-52-7].

IT 88552-48-1 88552-49-2 88552-51-6

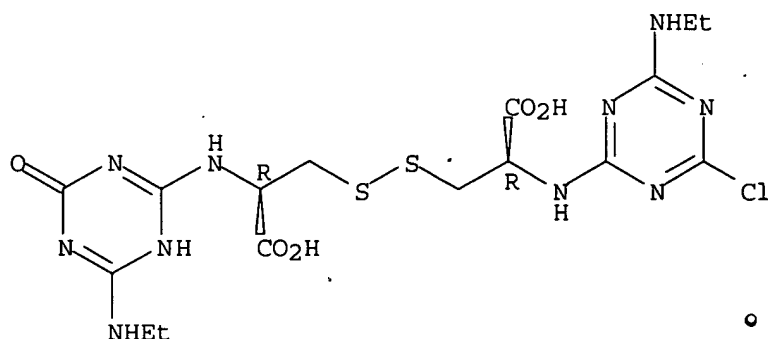
RL: BIOL (Biological study)

(chloroethylaminotriazinylcystine metabolite in cucumber)

RN 88552-48-1 HCAPLUS

CN L-Cystine, N-[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]-N'-[6-(ethylamino)-1,4-dihydro-4-oxo-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

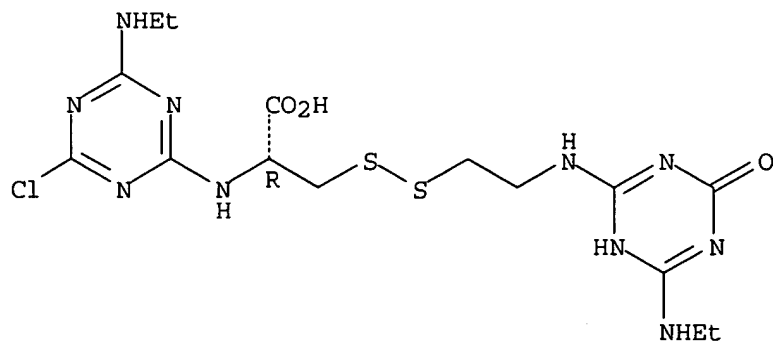
Absolute stereochemistry.



RN 88552-49-2 HCAPLUS

CN L-Alanine, N-[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]-3-[[2-[[6-(ethylamino)-1,4-dihydro-4-oxo-1,3,5-triazin-2-yl]amino]ethyl]dithio]- (9CI) (CA INDEX NAME)

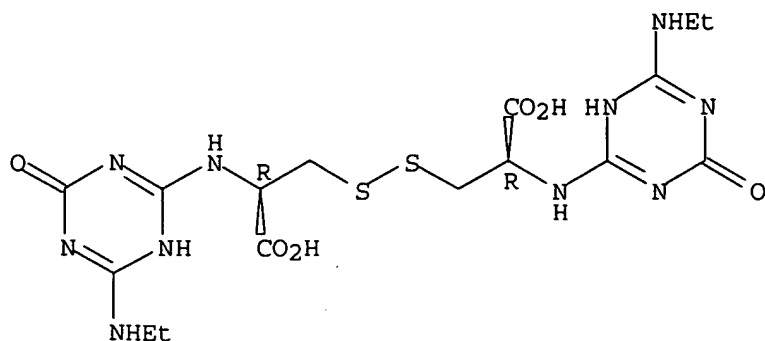
Absolute stereochemistry.



RN 88552-51-6 HCAPLUS

CN L-Cystine, N,N'-bis[6-(ethylamino)-1,4-dihydro-4-oxo-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



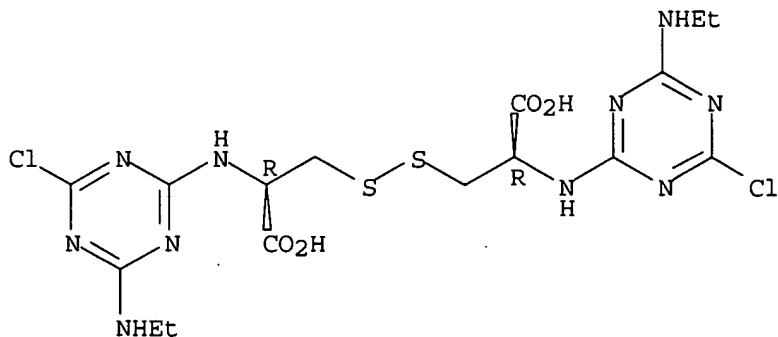
IT 88552-50-5

RL: PRP (Properties)
(degradation of, by cucumber)

RN 88552-50-5 HCAPLUS

CN L-Cystine, N,N'-bis[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1980:446607 HCAPLUS

DOCUMENT NUMBER: 93:46607

TITLE: Optically active S-triazine: preparation of
α-(2-anilino-4-amino-S-triazin-6-ylamino)-β-
thiolpropionic acid

AUTHOR(S): Watanabe, Nobuo; Mitsumoto, Isao; Kato, Tadashi;
Usami, Takashi

CORPORATE SOURCE: Tokyo Natl. Tech. Coll., Tokyo, Japan

SOURCE: Tokyo Kogyo Koto Senmon Gakko Kenkyu Hokokusho (
1979), 11, 83-6

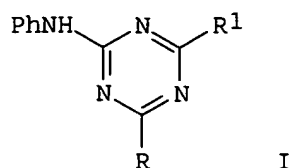
CODEN: TKSHDL; ISSN: 0286-0503

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

OTHER SOURCE(S): CASREACT 93:46607

GI



AB The title triazine derivative I [R = NH₂, R₁ = NHCH(CH₂SH)CO₂H] was prepared by amination of cyanuric chloride with aniline in acetone at 0-5° to give 96.7% I (R = R₁ = Cl) (II), amination of II with L-(-)-cysteine in acetone at 40-50° to give 86.2% I [R = Cl, R₁ = NHCH(CH₂SH)CO₂H], followed by amination with NH₄OH 2 h at 80-90° (in 83.3% yield).

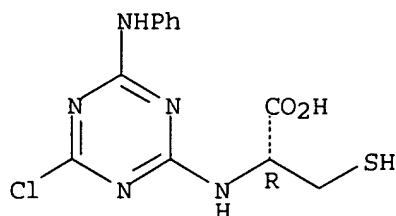
IT **74148-69-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)

RN 74148-69-9 HCAPLUS

CN L-Cysteine, N-[4-chloro-6-(phenylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



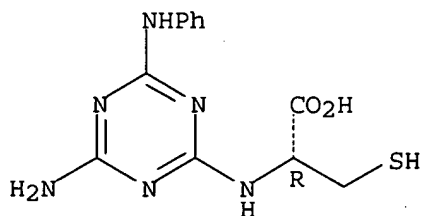
IT **74148-70-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 74148-70-2 HCAPLUS

CN L-Cysteine, N-[4-amino-6-(phenylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1980:6900 HCAPLUS

DOCUMENT NUMBER: 92:6900

TITLE: Mononuclear molybdenum(V) complexes of a cysteinyl

peptide
 AUTHOR(S): Garner, C. David; Mabbs, Frank E.; Richens, David T.
 CORPORATE SOURCE: Chem. Dep., Univ. Manchester, Manchester, UK
 SOURCE: Journal of the Chemical Society, Chemical
 Communications (1979), (9), 415-17
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The title complexes were prepared by reactions of MoOCl₃(THF)₂ (I) with a
 peptide containing cysteinyl and cystinyl groups at .apprx.20°; ESR
 characteristics and certain chemical behavior observed resemble those of the Mo
 centers in nitrate reductase and other molybdoenzymes. A mononuclear
 complex was also obtained by reaction of I with a peptide containing cysteinyl
 and histidine groups.
 IT **72068-28-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and ESR of)
 RN 72068-28-1 HCAPLUS
 CN Molybdenum, trichloro[ethyl N-[(phenylmethoxy)carbonyl]-L-cysteinyl-L-
 cysteinate bimol. (1→1')-disulfide]oxo-, (OC-6-21)- (9CI) (CA
 INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT **72063-46-8P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 72063-46-8 HCAPLUS
 CN Molybdenum(1+), dichloro[ethyl N-[(phenylmethoxy)carbonyl]-L-cysteinyl-L-
 cysteinate bimol. (1→1')-disulfide]dioxo-, (OC-6-22)- (9CI) (CA
 INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

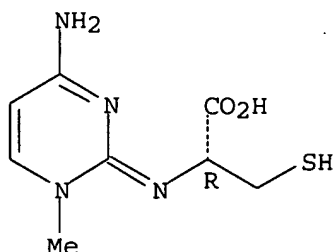
L22 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1978:132899 HCAPLUS
 DOCUMENT NUMBER: 88:132899
 TITLE: Nucleophilic substitution at C-2 of S-alkylated
 2-thiocytidines by cysteine and lysine. A new method
 for specific covalent linking of peptides to nucleic
 acids
 AUTHOR(S): Kroeger, Manfred; Cramer, Friedrich
 CORPORATE SOURCE: Abt. Chem., Max-Planck-Inst. Exp. Med., Goettingen,
 Fed. Rep. Ger.
 SOURCE: Bioorganic Chemistry (1977), 6(4), 431-41
 CODEN: BOCMBM; ISSN: 0301-4622
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB S-alkylated 2-thiocytidine can be substituted at C2 by nucleophilic
 agents. This reaction was investigated with model compds. as well as with
 tRNA by using cysteine and lysine to develop a new affinity label linking
 covalently tRNA and a protein. Reaction with N-protected cysteine gives
 2-S-alkylpyrimidines, whereas unprotected cysteine yields an
 N-alkylpyrimidine after intramol. substitution. With the ε-amino
 group of lysine a fast replacement at C2 is observed, leading to an unstable
 2-N-alkylpyrimidine. All products were characterized chemical and
 spectroscopically.

IT **66065-59-6P 66065-64-3P**
 RL: PREP (Preparation)
 (preparation of, nucleate-peptide conjugation in relation to)

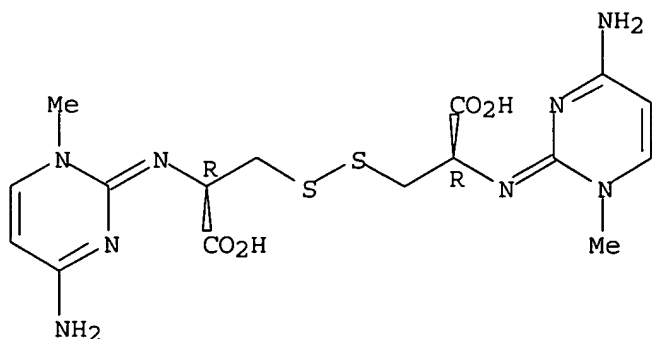
RN 66065-59-6 HCAPLUS
 CN L-Cysteine, N-(1,4-dihydro-4-imino-1-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



RN 66065-64-3 HCAPLUS
 CN L-Cystine, N,N'-bis(1,4-dihydro-4-imino-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



L22 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1976:12263 HCAPLUS
 DOCUMENT NUMBER: 84:12263
 TITLE: Metabolic disposition of carbon-14-labeled azathioprine in the dog
 AUTHOR(S): De Miranda, Paulo; Beacham, Lowrie M., III; Creagh, Teresa H.; Elion, Gertrude B.
 CORPORATE SOURCE: Wellcome Res. Lab., Burroughs Wellcome Co., Research Triangle Park, NC, USA
 SOURCE: Journal of Pharmacology and Experimental Therapeutics (1975), 195(1), 50-7
 CODEN: JPETAB; ISSN: 0022-3565
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB The metabolic disposition of the methylnitroimidazole moiety of azathioprine (I) [446-86-6], labeled with 14C in carbons 4 and 5 of this imidazole ring, was investigated in the dog. The administration of the radioactive drug (10 mg/kg, orally) was followed, after absorption, by a

rapid uptake of the radioactivity into the blood cells, with subsequent redistribution to the plasma. The total urinary excretion of ^{14}C was 41.6% in 32 hrs. Anion exchange and high-pressure liquid chromatog. of the urine revealed a large number of ^{14}C -containing metabolites. These included unmetabolized I, 1-methyl-4-nitro-5-(N-acetyl-S-cysteinyl)imidazole [51052-82-5], 1-methyl-4-nitro-5-thioimidazole [6339-54-4] and several compds. with ultraviolet absorption spectra similar to 5-substituted amino-1-methyl-4-nitroimidazoles. The most prominent of these was a highly acidic metabolite which was found to be identical in chemical, chromatog. and spectral properties with N,N'-[5-(1-methyl-4-nitroimidazolyl)cystine [57350-55-7]. This metabolite as well as 1-methyl-4-nitro-5-(N-acetyl-S-cysteinyl)imidazole and 1-methyl-4-nitro-5-thioimidazole were also identified in the urine of a dog given 1-methyl-4-nitro-5-(S-glutathionyl)-imidazole [36892-55-4] (10 mg/kg, i.v.) suggesting that the latter compound is an intermediate in the formation of these urinary metabolites. The profile of the methylnitroimidazole urinary metabolites in the dog was similar to that in man and different from that in the rat. A metabolic pathway for the formation of these metabolites in the dog is proposed.

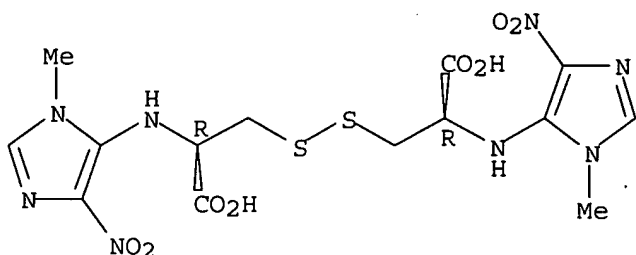
IT 57350-55-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as azathioprine metabolite)

RN 57350-55-7 HCAPLUS

CN L-Cystine, N,N'-bis(1-methyl-4-nitro-1H-imidazol-5-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1975:564565 HCAPLUS

DOCUMENT NUMBER: 83:164565

TITLE: Methods of peptide sequencing. II. Cyclization of N-2-amino-6-nitrophenyl and N-3-amino-2-pyridyl derivatives of amino acids and peptides

AUTHOR(S): Johnstone, Robert A. W.; Povall, T. Jeffrey; Entwistle, Ian D.

CORPORATE SOURCE: Robert Robinson Lab., Univ. Liverpool, Liverpool, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1975), (14), 1424-7
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Treatment of amino acid and peptide Me ester hydrochlorides with 2,6-(O₂N)₂C₆H₃F on 2-fluoro-3-nitropyridine (I) gave the corresponding N-nitroaryl derivs. Reduction of these derivs. by transfer catalysis and

cyclization of the N-aminoaryl derivs. formed gave, in the peptide case, release of the peptide minus its N-terminal amino acid residue. This cycle of reactions was used to obtain a partial sequence of amino acids in a peptide. Thus the hydrochloride of the octapeptide, H-Glu(OMe)-Glu(OMe)-Ala-Glu(OMe)-Glu(OMe)-Ala-Tyr-Gly-OMe on reaction with I gave the corresponding N-nitroaryl derivative which on reduction and cyclization

gave initially II, and the corresponding peptide residue. Derivatization and reduction-cyclization steps were repeated with the residue to give successively the pyridopyrazines from Glu(OMe), Ala, and Glu(OMe) twice. At the sixth cycle, no pyridopyrazine corresponding to alanine was detected.

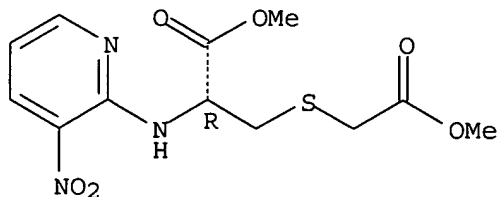
IT 57461-52-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 57461-52-6 HCAPLUS

CN L-Cysteine, S-(2-methoxy-2-oxoethyl)-N-(3-nitro-2-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1974:615 HCAPLUS

DOCUMENT NUMBER: 80:615

TITLE: Atrazine metabolism in sorghum. Catabolism of the glutathione conjugate of atrazine

AUTHOR(S): Lamoureux, Gerald L.; Stafford, Lester E.; Shimabukuro, Richard H.; Zaylskie, Richard G.

CORPORATE SOURCE: Metab. Radiat. Res. Lab., Agric. Res. Serv., Fargo, ND, USA

SOURCE: Journal of Agricultural and Food Chemistry (1973), 21(6), 1020-30

CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The major pathway of atrazine (I) [1912-24-9] metabolism in intact sorghum involved the following steps: I .far. S-(4-ethylamino-6-isopropylamino-s-triazinyl-2)glutathione [24429-05-8] .far. γ -glutamyl-S-(4-ethylamino-6-isopropylamino-s-triazinyl-2)cysteine [24428-76-0] .far. S-(4-ethylamino-6-isopropylamino-s-triazinyl-2)cysteine (II) [43171-11-5] .far. N-(4-ethylamino-6-isopropylamino-s-triazinyl-2)cysteine (III) [43171-12-6] .far. N-(4-ethylamino-6-isopropylamino-s-triazinyl-2)anthione (IV) [49564-63-8]. From 40 to 87% of the I entering sorghum through the roots was metabolized via this pathway. Apparently I could also be metabolized via this route after N-dealkylation. The conversion of II to III was a nonenzymic rearrangement. This was the 1st reported occurrence of II, IV, 2-hydroxy-4-amino-6-isopropylamino-s-triazine [19988-24-0], and 2-hydroxy-4,6-diamino-s-triazine [645-92-1] in sorghum.

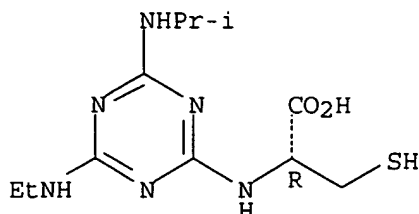
IT 43171-12-6 49564-63-8

RL: FORM (Formation, nonpreparative)
(formation of, as atrazine metabolite in sorghum)

RN 43171-12-6 HCAPLUS

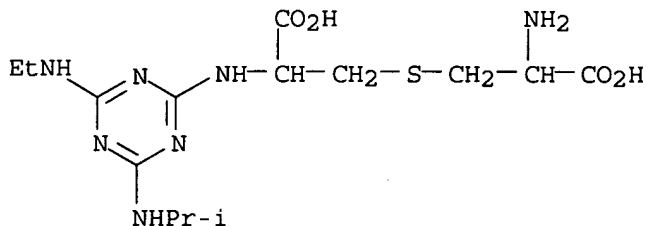
CN L-Cysteine, N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 49564-63-8 HCAPLUS

CN L-Cysteine, S-(2-amino-2-carboxyethyl)-N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)



L22 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:543389 HCAPLUS

DOCUMENT NUMBER: 79:143389

TITLE: Atrazine metabolism in sorghum. Chloroform-soluble intermediates in the N-dealkylation and glutathione conjugation pathways

AUTHOR(S): Shimabukuro, Richard H.; Walsh, Wendy C.; Lamoureux, Gerald L.; Stafford, Lester E.

CORPORATE SOURCE: State Univ. Stn., Agric. Res. Serv., Fargo, ND, USA

SOURCE: Journal of Agricultural and Food Chemistry (

1973), 21(6), 1031-6

CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two unrelated metabolites of atrazine (I) [1912-24-9], 2-chloro-4,6-diamino-s-triazine (II) [3397-62-4], and N,N'-bis(4-ethylamino-6-isopropylamino-s-triazinyl-2)cystine (III) [43171-17-1], were isolated from sorghum plants treated with 10-5-10-4M I solns. for 5-20 days. II was produced by complete N-dealkylation of I, and no longer inhibited the Hill reaction or cyclic and noncyclic photophosphorylation in isolated pea chloroplasts. The presence of III suggests that I was metabolized by the glutathione pathway to its lanthione conjugate. III is not necessarily present in the plant as the dimer, however the N-cysteine monomer may dimerize in vivo.

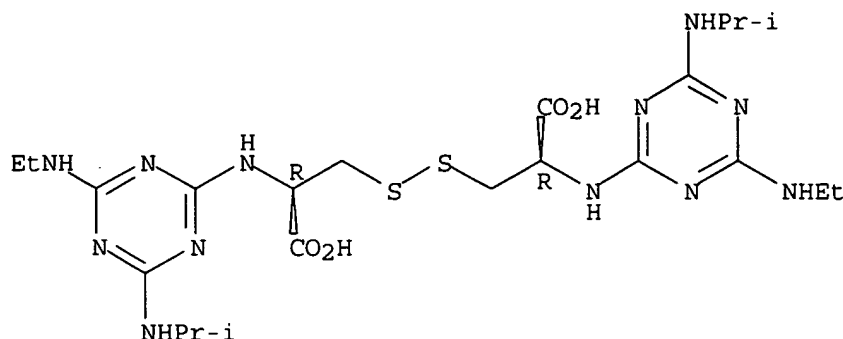
IT 43171-17-1

RL: BIOL (Biological study)
(as atrazine metabolite, in sorghum)

RN 43171-17-1 HCAPLUS

CN L-Cystine, N,N'-bis[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1972:415409 HCAPLUS

DOCUMENT NUMBER: 77:15409

TITLE: Metabolism of simazine and atrazine by wild cane

AUTHOR(S): Thompson, Lafayette, Jr.

CORPORATE SOURCE: Dep. Agron., Univ. Kentucky, Lexington, KY, USA

SOURCE: Weed Science (1972), 20(2), 153-5

CODEN: WEESA6; ISSN: 0043-1745

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Atrazine (I) [1912-24-9] and simazine (II) [122-34-9] were metabolized in the wild cane (*Sorghum bicolor*) by hydroxylation and peptide conjugation. The wild cane absorbed in vivo equal amts. of I and II. The plants metabolized 70% of the I and 30% of the II absorbed and translocated to the shoot during 24 hr. The major metabolites formed were hydroxy derivatives and very hydrophilic peptide conjugates, such as S-(4-ethylamino-6-isopropylamino-s-triazin-2-yl)glutathione. The wild cane formed peptide conjugates of I more rapidly than of II, but hydroxylation of I and II occurred at the same rate.

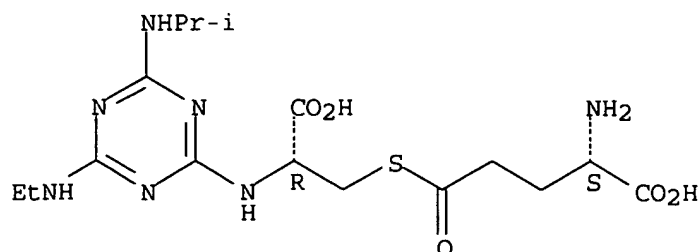
IT 36959-29-2

RL: FORM (Formation, nonpreparative)
(formation of, in atrazine metabolism by *Sorghum bicolor*)

RN 36959-29-2 HCAPLUS

CN L-Cysteine, N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]-, 1-hydrogen glutamate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 23 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1972:405775 HCAPLUS

DOCUMENT NUMBER: 77:5775

TITLE: Nitro heteroaromatic derivatives of amino acids and peptides. III. Application of ultraviolet-visible absorption and circular dichroism to N-(3-nitro-2-pyridyl)amino acids

AUTHOR(S): Toniolo, C.; Nisato, D.; Biondi, L.; Signor, A.

CORPORATE SOURCE: Inst. Org. Chem., Univ. Padova, Padua, Italy

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1972), (9-10), 1179-81

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Uv-visible absorption and CD curves were recorded for 23 N-(3-nitro-2-pyridyl)amino acids, e.g., N-(3-nitro-2-pyridyl)alanine. The 420 nm CD band was correlated with the absolute configuration of N-(3-nitro-2-pyridyl)amino acids, thus allowing determination of the absolute configurations of the N-terminal amino acids of peptides.

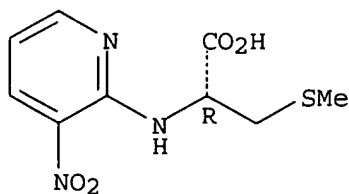
IT 36976-96-2 36976-97-3

RL: PRP (Properties)
(circular dichroism of)

RN 36976-96-2 HCAPLUS

CN L-Cysteine, S-methyl-N-(3-nitro-2-pyridinyl)- (9CI) (CA INDEX NAME)

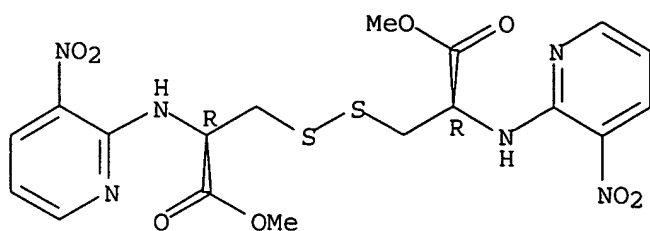
Absolute stereochemistry.



RN 36976-97-3 HCAPLUS

CN L-Cystine, N,N'-bis(3-nitro-2-pyridinyl)-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 24 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1972:141296 HCAPLUS

DOCUMENT NUMBER: 76:141296

TITLE: Nitroheteroaromatic derivatives of amino acids and peptides. II. Optical properties of 3,5-dinitro-2-pyridyl-L-amino acids and related compounds

AUTHOR(S): Nisato, Dino; Marzotto, Armando; De Pieri, Gianfranco; Signor, Angelo

CORPORATE SOURCE: Ist. Chim. Org., Univ. Padova, Padua, Italy

SOURCE: Gazzetta Chimica Italiana (1971), 101(11), 805-14

CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Amino and pyridyl amino acid derivs., prepared by a coupling reaction of L-amino acids with 2-chloro-3,5-dinitropyridine (I) show a rotation shift varying from 70 to 100° (>300° for proline). Thus, I was added to alanine and Na₂CO₃ at 40° to give 94% II. Similarly prepared were 3,5-dinitro-2-pyridyl derivs. of arginine, asparagine, aspartic acid, cysteine, glutamine, hydroxyproline, histidine, lysine, phenylalanine, proline, serine, threonine, tryptophan, and glutathione.

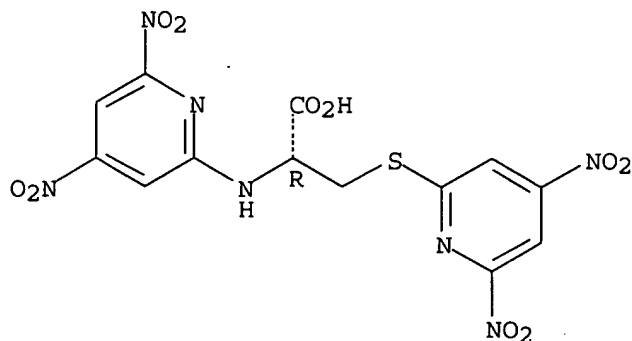
IT 35899-61-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35899-61-7 HCAPLUS

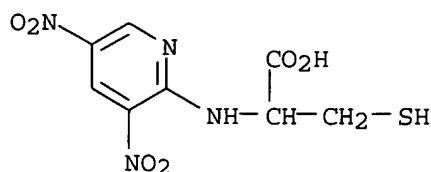
CN L-Cysteine, N,S-bis(4,6-dinitro-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

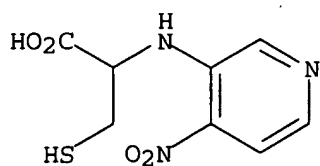


L22 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

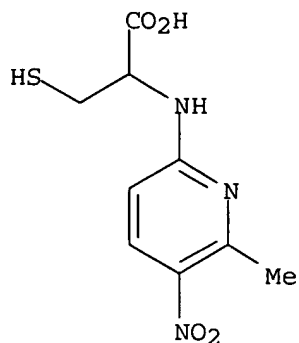
ACCESSION NUMBER: 1968:459052 HCAPLUS
 DOCUMENT NUMBER: 69:59052
 TITLE: Reactivity of fluoronitropyridines. II. Derivates of fluoronitropyridines
 AUTHOR(S): Talik, T.; Talik, Z.
 CORPORATE SOURCE: Hochsch. Wirtschaftsfragen, Wroclaw, Pol.
 SOURCE: Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques (1968), 16(1), 7-12
 CODEN: BAPCAQ; ISSN: 0001-4095
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB Fluoronitropyridines and their derivs. were prepared as previously described (T. Talik and Z. Talik, 1964-7). Their reactivity could be compared as follows: 3,5-dinitro-2-fluoropyridine > 3-fluoro-4-nitropyridine N-oxide > 3-fluoro-5-methyl-4-nitropyridine N-oxide > 2-fluoropyridines with a Me group in the 3, 4, 5, or 6 position and a nitro group in the 3 or 5 position > 3-fluoro-4-nitropyridine > 3-fluoro-2-methyl-4-nitropyridine N-oxide > 2-fluoro-4-nitropyridine > 2,6-dimethyl-3-fluoro-4-nitropyridine N-oxide.
 IT 19339-98-1P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 19339-98-1 HCAPLUS
 CN Cysteine, N-(3,5-dinitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)



L22 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1968:459051 HCAPLUS
 DOCUMENT NUMBER: 69:59051
 TITLE: Reactivity of fluoronitropyridines. III. Conversion of fluoronitropyridines with amino acids
 AUTHOR(S): Talik, T.; Talik, Z.
 CORPORATE SOURCE: Hochsch. Wirtschaftsfragen, Wroclaw, Pol.
 SOURCE: Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques (1968), 16(1), 13-16
 CODEN: BAPCAQ; ISSN: 0001-4095
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB 3-Fluoro-4-nitropyridine, its N-oxide and 2-fluoro-5-nitro-6-methylpyridine form crystalline derivs. of the amino acids, which show variable resistance to hydrolysis. They have been used in the quant. study of casein hydrolyzates.
 IT 13505-11-8P 18710-42-4P 19367-19-2P
 19367-37-4P 19392-01-9P 19392-17-7P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 13505-11-8 HCAPLUS
 CN Cysteine, N-(4-nitro-3-pyridyl)-, DL- (8CI) (CA INDEX NAME)

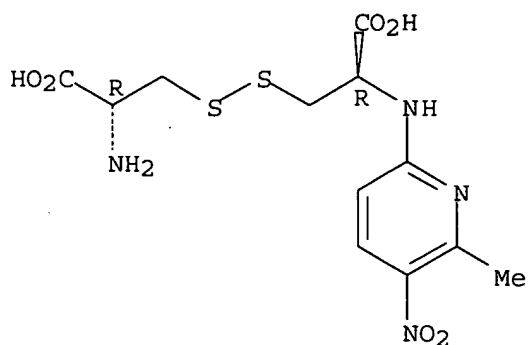


RN 18710-42-4 HCAPLUS
CN Cysteine, N-(6-methyl-5-nitro-2-pyridyl)-, DL- (8CI) (CA INDEX NAME)



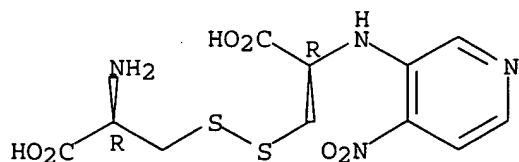
RN 19367-19-2 HCAPLUS
CN Cystine, N-(6-methyl-5-nitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



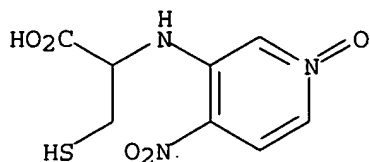
RN 19367-37-4 HCAPLUS
CN Cystine, N-(4-nitro-3-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 19392-01-9 HCAPLUS

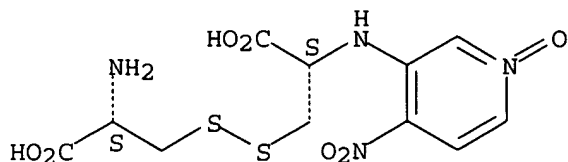
CN Cysteine, N-(4-nitro-3-pyridyl)-, 1-oxide, DL- (8CI) (CA INDEX NAME)



RN 19392-17-7 HCAPLUS

CN Cystine, N-(4-nitro-1-oxido-3-pyridinyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L22 ANSWER 27 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1968:410337 HCAPLUS

DOCUMENT NUMBER: 69:10337

TITLE: Synthesis and properties of 2-fluoro-3,5-dinitropyridine

AUTHOR(S): Talik, Tadeusz; Talik, Zofia

CORPORATE SOURCE: Wyzsza Szkola Ekon., Wroclaw, Pol.

SOURCE: Roczniki Chemii (1967), 41(9), 1507-11

CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB 3,5-Dinitropyridine-2-diazonium fluoroborate (prepared at 0° during 2 hrs. from 75 ml. 48% HF, 35 g. H3BO3, and 6 g. 2-amino-3,5-dinitropyridine, and 9 g. NaNO2) was neutralized with solid (NH4)2CO3 to pH 5 and the whole extracted with Et2O and worked up to give 2.7 g. 2-fluoro-3,5-dinitropyridine (I), m. 64° (C6H6-ligroine). Heating 0.2 g. I 1 min. in 2 ml. H2O led to 2-hydroxy-3,5-dinitropyridine, m. 176°. I refluxed 2 hrs. in MeOH yielded quant. 2-methoxy-3,5-dinitropyridine, m. 92°. Similarly prepared was 2-ethoxy-3,5-dinitropyridine, m. 71°. A mixture of 0.3 g. I, 2 ml. EtOH, and 0.5 g. PhNH2 afforded quant. 2-anilino-3,5-dinitropyridine, m. 152°. Similarly prepared was 2-phenylhydrazino-3,5-dinitropyridine, m. 143°. Heating a mixture of 0.2 g. thiourea and 0.2 g. I in 3 ml. EtOH 2 min., or 0.2 g. I, 0.2 g. MeCSNH2, and 0.2 g. NaHCO3 in 3 ml. EtOH led in both cases to a 50% yield of bis(3,5-dinitro-2-pyridyl) sulfide, m. 164°. A solution of 0.3 g. DL-threonine and 0.42 g. NaHCO3 in 5 ml. H2O was added to 0.47 g. I in 5 ml. EtOH, and the whole kept 5 min. at room temperature, acidified with dilute HCl, and concentrated to give 0.6 g. N-(3,5-dinitro-2-pyridyl)-DL-threonine, m. 121°. Similarly prepared were the following N-(3,5-dinitro-2-pyridyl) amino acid derivs. (amino acid, m.p., and % yield given): L-glutamic, 164°, 89; DL-cysteine, 159°, 82.9; and L-cystine, 120°, 34.7.

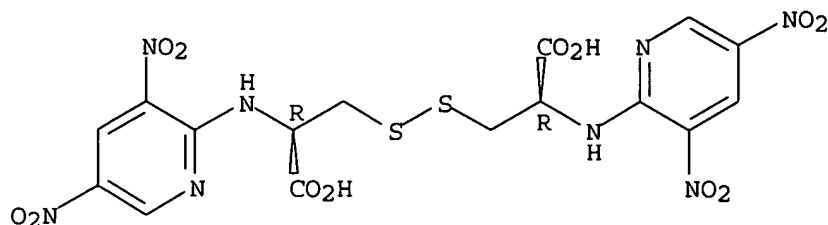
IT 18710-40-2P 19339-98-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 18710-40-2 HCAPLUS

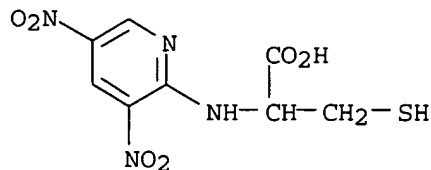
CN Cystine, N,N'-bis(3,5-dinitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 19339-98-1 HCAPLUS

CN Cysteine, N-(3,5-dinitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)



L22 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1968:403121 HCAPLUS

DOCUMENT NUMBER: 69:3121

TITLE: 2-Fluoro-5-nitro-6-methylpyridine. I. Reactions with amino acids

AUTHOR(S): Talik, Zofia; Brekiesz-Lewandowska, Barbara

CORPORATE SOURCE: Wyzsza Szkoła Ekon, Wrocław, Pol.

SOURCE: Roczniki Chemii (1967), 41(12), 2095-9

CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Syntheses of the title compound (I) and 23 amino acid derivs. were reported. Thus, 10 g. of 2-amino-5-nitro-6-methylpyridine was added at 0° to a solution of 48 g. H3BO3 in 100 ml. 48% HF followed by diazotization 1.5 hrs., with 15 g. solid NaNO2 and the whole stirred 20 min., neutralized with solid NH4HCO3, and steam distilled to give 4 g. I, b5 85°. A mixture of 0.39 g. I, 7 ml. EtOH, 5 ml. H2O, 0.42 g. NaHCO3, and 0.0025 mole of an amino acid refluxed 10 min. until the mixture became clear, was evaporated

and acidified with dilute HCl to afford the following N-(5-nitro-6-methyl-2-pyridyl) amino acid derivs. (amino acid, m.p., and % yield given):

glycine, 217° (decomposition), 70.4; DL-serine, 169° (decomposition),

56.6; DL-cysteine, 98°, 68.3; DL-α-alanine, 151°,

69.3; β-alanine, 163°, 86.7; DL-asparagine, 187°

(decomposition), 72.7; DL-threonine, 170° (decomposition), 61.2; DL-proline,

131°, 77.7; DL-hydroxyproline, 174°, 87.6; DL-glutamic acid,

174°, 69; L-valine, 144°, 84.8; DL-norvaline, 112°,

30.8; DL-methionine, 132°, 60.5; L-histidine, 159°, 40.2;

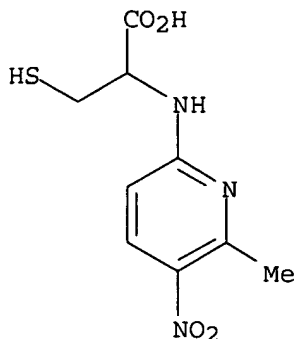
DL-leucine, 75°, 87.6; DL-isoleucine, 106°, 29.2;
DL-norleucine, 69°, 80.3; DL-lysine, 118°, 76; DL-arginine,
232° (decomposition), 88.3; D-phenylalanine, 90°, 91.6;
L-tyrosine, 204° (decomposition), 73.8; L-tryptophan, 126°, 91.7;
L-cystine, 175° (decomposition), 60.9.

IT 18710-42-4P 18710-61-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 18710-42-4 HCAPLUS

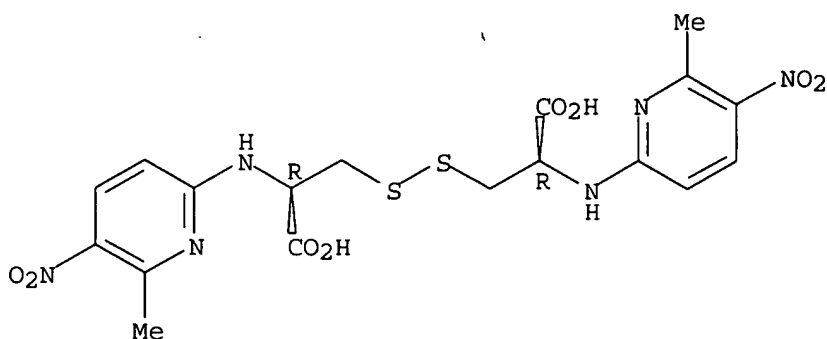
CN Cysteine, N-(6-methyl-5-nitro-2-pyridyl)-, DL- (8CI) (CA INDEX NAME)



RN 18710-61-7 HCAPLUS

CN Cystine, N,N'-bis(6-methyl-5-nitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:11165 HCAPLUS

DOCUMENT NUMBER: 66:11165

TITLE: 3-Fluoro-4-nitropyridine

AUTHOR(S): Talik, Tadeusz; Talik, Zofia

CORPORATE SOURCE: Wyzsza Szkola Ekon., Wroclaw, Pol..

SOURCE: Roczniki Chemii (1966), 40(7/8), 1187-93

CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Preparation and reaction of 3-fluoro-4-nitropyridine (I) with amines and amino acids were described. A solution of 5 g. 3-fluoro-4-aminopyridine in 15 ml.

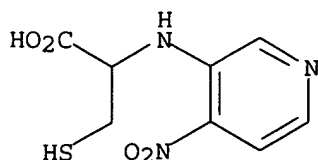
concentrated H₂SO₄ was added at 0° to persulfuric acid (prepared from 60 ml. 20% oleum and 40 ml. 30% H₂O₂), the whole was kept 24 hrs. at room temperature, then poured into ice, neutralized with NH₄HCO₃, and extracted with CHCl₃. The extract evaporated and the residue steam distilled gave 4 g. I, b₅ 62-4°. A solution of 2 g. I in 30 ml. NH₃-saturated MeOH autoclaved 7 hrs. at 130° afforded 1.5 g. 3-amino-4-nitropyridine, m. 140° (H₂O). A solution of 1 g. I and 2 g. PhNH₂ in 5 ml. EtOH refluxed 1 hr. yielded 79.2% 3-phenylamino-4-nitropyridine, m. 116° (alc.). Similarly prepared were: 3-ethylamino-4-nitropyridine, m. 96° (H₂O); 3-(ethanolamino) 4-nitropyridine, m. 129° (H₂O). A mixture of 0.5 g. KOH, 4 ml. H₂O, 1 ml. 30% H₂O₂, and 0.5 g. I kept 15 min. until the exothermic reaction ceased and acidified with dilute HCl gave 0.4 g. 3-hydroxy-4-nitropyridine, m. 132° (H₂O). A solution of 1.42 g. I, and MeONa (prepared from 0.23 g. Na and 25 ml. MeOH) kept 1 hr. at room temperature and worked up, yielded 79.5% 3-methoxy-4-nitropyridine, m. 46° (ligroine). Similarly prepared was 89.3% 3-ethoxy-4-nitropyridine, m. 40°. A series of 4-nitro-3-pyridyl amino acid (II) derivs. was prepared according to the following procedure. A solution of 0.005 mole amino acid, 0.01 mole NaHCO₃ (or 0.015 mole for dibasic amino acids) in 5 ml. H₂O was stirred with 0.005 mole I in 15 ml. EtOH, then refluxed 15 min. and evaporated in vacuo. The residue acidified with diluted HCl, filtered, and recrystd. afforded the following II (amino acid component, m.p., and % yield given): glycine, 184° (H₂O), 81.2; DL-serine, 196° (H₂O), 44.1; DL-cysteine (III), 154°, 65.8; D,L-α-alanine, 199° (EtOH-H₂O), 70.5; β-alanine, 208° (EtOH-H₂O), 70.5; DL-aspartic acid, 185° (H₂O), 54.9; DL-asparagine (IV), 180° (H₂O), 55.1; DL-threonine, 195° (H₂O), 58.1; DL-proline, 124° (H₂O-EtOH), 75.9; DL-glutamic acid, 162° (H₂O), 59.5; L-glutamine (V), 163° (H₂O), 41; DL-valine, 154° (H₂O-EtOH), 75.3; DL-norvaline, 160° (H₂O-EtOH), 58.6; DL-methionine, 126° (H₂O-EtOH), 59; L-histidine (VI), 242° (H₂O), 50.5; L-leucine, 130° (H₂O-EtOH), 71.1; DL-isoleucine, 184° (H₂O-EtOH), 71.1; DL-norleucine, 147° (H₂O-EtOH), 55.3; L-lysine, 145° (H₂O-EtOH), 52.2; DL-arginine, 219° (H₂O-EtOH), 47.3; D-phenylalanine, 189° (H₂O-EtOH), 55.7; DL-tyrosine, 108° (H₂O-EtOH), 59.4; L-tryptophan (VII), 203°, 89.2; L-cystine, 166° (EtOH), 38. III and VII were purified by dissolving in aqueous Na-HCO₃, shaking with active C, and acidifying with dilute HCl. IV-VI were isolated from the reaction mixture when acidified with HCl at pH 6-7.

IT 13505-11-8P 15445-33-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 13505-11-8 HCAPLUS

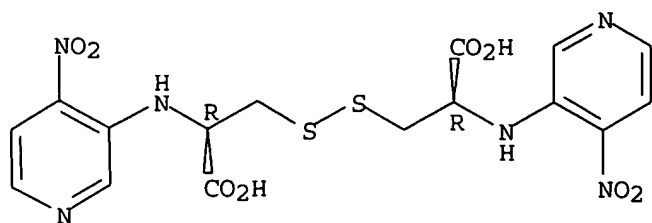
CN Cysteine, N-(4-nitro-3-pyridyl)-; DL- (8CI) (CA INDEX NAME)



RN 15445-33-7 HCAPLUS

CN Cystine, N,N'-bis(4-nitro-3-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 30 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1964:461919 HCAPLUS

DOCUMENT NUMBER: 61:61919

ORIGINAL REFERENCE NO.: 61:10769e-h

TITLE: 3-Fluoro-4-nitropyridine N-oxide. II. Reactions with amino acids

AUTHOR(S): Talik, Tadousz; Talik, Zofia

CORPORATE SOURCE: School of Econ., Wroclaw, Pol.

SOURCE: Roczniki Chemii (1964), 38(5), 785-8

CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Cf. CA 61, 10653c. 3-Fluoro-4-nitropyridine N-oxide (I) readily formed crystalline derivs. with amino acids in high yields. Thus, 0.005 mole of amino acid and 0.01 mole NaHCO₃ in 10 ml. H₂O warmed at 60° until the solution became clear, treated with a warm (60°) solution of 0.005 mole I in 15 ml. EtOH, kept 10 min. at room temperature, excess alc. evaporated in vacuo,

and the residue treated with dilute HCl afforded the crystalline derivative The

reaction products of I with lysine, cystine, cysteine, and tryptophan were purified by dissolving in aqueous NaHCO₃, stirring with C, and precipitating with dilute

HCl. The reaction product of I with histidine was dried in vacuo over P₂O₅. In the case of dibasic amino acids, 0.015 mole was used. The following addition products of I with the cited amino acid were prepared (m.p., and % yield given): glycine, 216°, 93.9; (±)serine, 212° (decomposition), 52.6; (±)-cysteine, 173° (decomposition), 61.7; (±)-α-alanine, 216° (decomposition), 87.1; β-alanine, 228° (decomposition), 78.4; (±)-aspartic acid, 214° (decomposition), 90.4; (±)-threonine, 203° (decomposition), 54; (±)-proline, 175° (decomposition), 80.8; (±)-glutamic acid, 205° (decomposition), 77.4; (±)-valine, 219° (decomposition), 76.7; (±)-norvaline, 168°, 69; (±)-methionine, 162°, 94.4; (±)-histidine, 199° (decomposition), 84.6; (-)-leucine, 182°, 89.2; (±)-isoleucine, 179°, 89.2; (±)-norleucine, 164°, 57.8; (±)-lysine, 185° (decomposition), 91.6; (±)-tyrosine, 145° (decomposition), 94.1; (±)-phenylalanine, 202° (decomposition), 99; (±)-tryptophan, 216° (decomposition), 83.5; (±)-cystine, 172° (decomposition), 46.6.

IT 819046-88-3, Cysteine, N-(4-nitro-3-pyridyl)-, oxide, DL- (preparation of)

RN 819046-88-3 HCAPLUS

CN Cysteine, N-(4-nitro-3-pyridyl)-, oxide, DL- (7CI) (CA INDEX NAME)

LUKTON: 09 / 600659

